

Crystalline Cu-Sn-S Framework for High Lithium Storage

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Supporting Information

Table S1. Crystallographic data and structure refinement for CTS

CTS	
Chemical formula	C ₂ N ₂ H ₁₆ OCu ₈ Sn ₃ S ₁₂
Formula mass	1349.278
Crystal system	Cubic
Space group	F-43c
<i>a</i> (Å)	18.040(2)
<i>b</i> (Å)	18.040(2)
<i>c</i> (Å)	18.040(2)
α (deg)	90.00
β (deg)	90.00
γ (deg)	90.00
V (Å ³)	5871.0(12)
<i>Z</i>	4
D _{cal} (g/cm ³)	3.116
Theta (deg)	3.19-27.00
GOF on F ²	1.118
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> >2σ(<i>I</i>)]	0.0374, 0.1058
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.0525, 0.1157

$$^aR_1 = \sum \left\| \mathbf{F}_o \right\| - \left\| \mathbf{F}_c \right\| / \sum \left\| \mathbf{F}_o \right\|. \quad ^bR_2 = \left[\sum w \left(\mathbf{F}_o^2 - \mathbf{F}_c^2 \right)^2 / \sum w \left(\mathbf{F}_o^2 \right)^2 \right]^{1/2}.$$

Table S2. A survey of electrochemical properties of Tin-based materials for LIBs

Electrode description	Cycling stability	Cycling stability	Ref.
SnS ₂ nanoparticles	293 mAh g ⁻¹ after 50 cycles at 50 mA g ⁻¹ (a capacity fade of 4.7 mAh g ⁻¹ per cycle)	55.6% of an initial capacity of 527 mAh g ⁻¹	1
SnS ₂ powder	400 mAh g ⁻¹ after 25 cycles at 50 mA g ⁻¹	66.6% of an initial capacity of 600 mAh g ⁻¹	2
SnO ₂ nanowires	300 mAh g ⁻¹ up to the 50th cycle	60% of the fifth-cycle capacity	3
SnO ₂ hollow structures	About 500 mAh g ⁻¹ at 100 mA g ⁻¹ after 40 cycles	43.8 % of an initial capacity of 1140 mAh g ⁻¹	4
2D-SnS ₂ nanoplates	583 mAhg 100mA g ⁻¹ after 30 cycles	85% of the 2nd-cycle capacity	5
SnS ₂ nanotables	168 mAh g ⁻¹ at 0.5 C after 200 cycles	60% of the initial capacity of 1250 mAh g ⁻¹	6

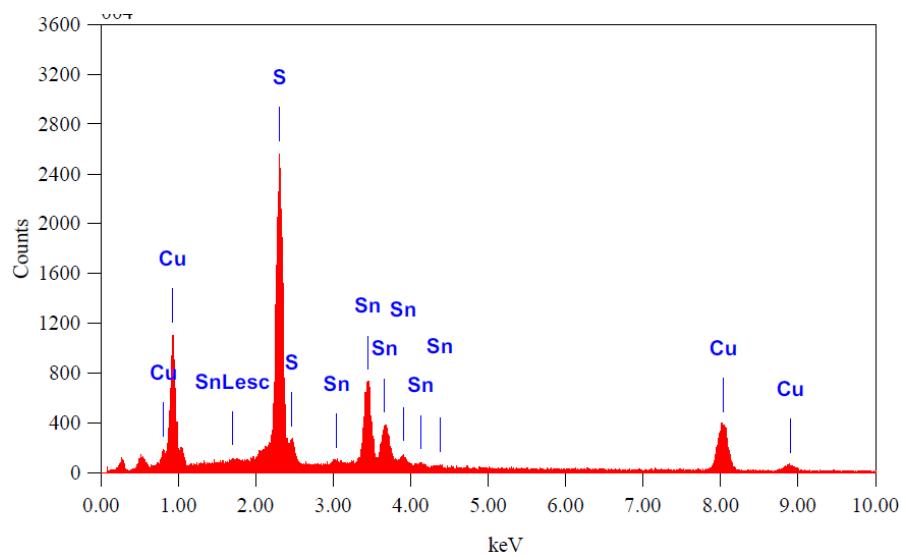


Figure S1. The energy dispersive X-ray (EDX) spectroscopy of CTS.

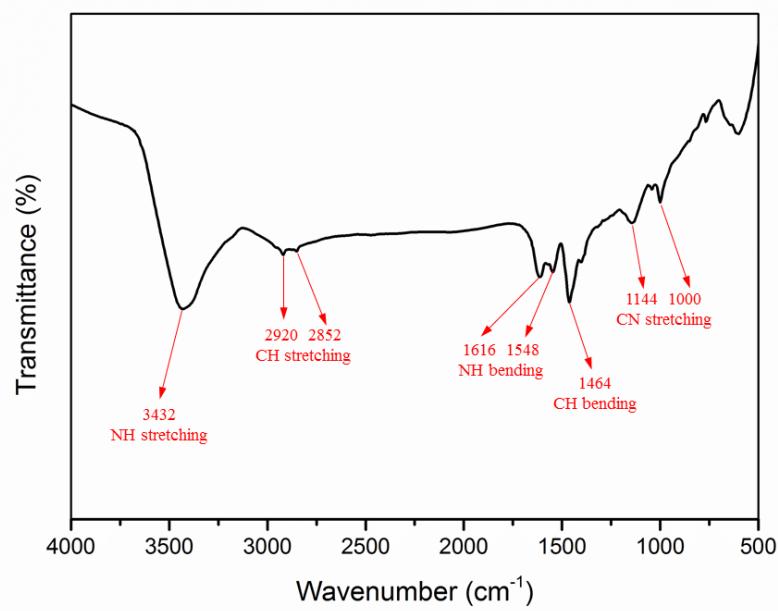


Figure S2. FTIR spectrum for CTS with the assignment of main absorption peaks.

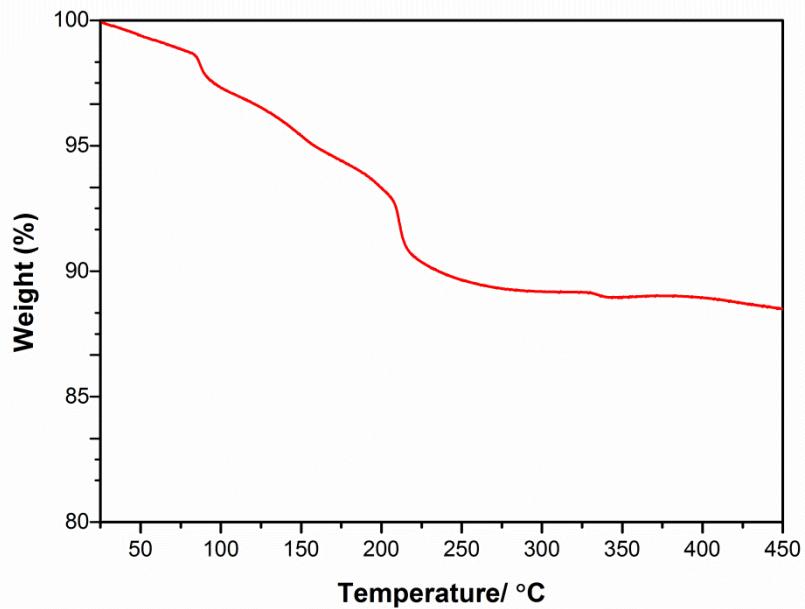


Figure S3. TGA curve for CTS.

References

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